

General expressions for the dispersion relation of acoustic radial (breathing) modes in cylinders and cylindrical shells of general anisotropic crystals

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Abstract

We present here a study of the radial modes for infinitely long cylinders and cylindrical shells of general anisotropic crystals. The elastic coefficients matrix includes twenty-one independent constants. We obtain expressions in closed form for the dispersion relation, valid for any anisotropic material. In the case of the lowest breathing mode of a thin cylindrical shell we obtain a simple analytical formula. This can be used to obtain a first estimate of the breathing mode frequency in nanotubes for any material.

I. INTRODUCTION

Cylindrical systems are frequently used as structural components in many engineering areas: aerospace, civil engineering, etc., and their vibration characteristics are obviously important for practical design.

The study of acoustic wave propagation in infinitely long homogeneous cylinders and cylindrical layers is a well established field from the initial studies of Pochhammer¹ and Chree^{2,3}. They developed exact solutions for torsional and longitudinal vibrations of infinitely long homogeneous isotropic solid cylinders with stress free faces. Gazis provided solutions for the acoustic wave propagation problem in homogeneous isotropic cylinders of infinite length⁴. Studies for orthotropic hollow and thick cylinders of infinite length, including nine independent elastic constants, were done by Mirsky⁵. Detailed discussions on these problems and more references can be found in Refs.6-8.

No general expressions for the dispersion relation of the acoustic waves in cylinders of general anisotropic crystals are available, to our knowledge, although it has been possible to obtain solutions in closed form for some particular kinds of modes and crystal systems. The radial (breathing) modes of cylinders have a much simpler form than a general vibrational mode, thus making them good candidates to try to obtain its dispersion relation for general anisotropic crystals.

On the other hand the study of carbon nanotubes (CNT) and nanowires of many other materials, belonging to different crystal systems, has increased the use of isotropic continuum models for cylinders and cylindrical shells⁹⁻¹³. In the case of transverse elastic isotropy (hexagonal crystals) formal expressions were given in Ref.14. In the case of general anisotropic crystals, a method developed in resonant ultrasound spectroscopy to get the free vibrational modes of inhomogeneous systems¹⁵⁻¹⁸, has been employed in several studies of acoustic modes in nanowires¹⁹⁻²².

Quite recently the acoustic modes in nanorods of different materials²³⁻²⁵ have been observed directly by optical methods. Other approaches in continuum media²⁶⁻²⁸ are also been used. This shows the interest in the study of the vibrational modes of nanotubes and nanowires.

Thus it is worthwhile to try to get expressions in closed form for the radial modes frequencies in cylinders and cylindrical shells of general anisotropic crystals.

We shall consider here an infinitely long cylinder, or cylindrical shell, of a general anisotropic material and we shall obtain the dispersion relation of the radial modes for these systems.

In Section II we present the formal equations leading to the dispersion relation and the comparison with other simpler cases. Conclusions are presented in Section III.

II. ACOUSTIC RADIAL MODES IN CYLINDERS AND CYLINDRICAL SHELLS OF GENERAL ANISOTROPIC CRYSTALS

We shall consider a general anisotropic crystal. The matrix of elastic coefficients will be given in this case by

$$C_{\alpha\beta} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \quad (1)$$

including twenty-one independent constants.

We shall consider a homogeneous thick cylinder of infinite length and radius R , or a homogeneous cylindrical shell of infinite length, inner radius a , outer radius b and thickness h ($b = a + h$). We shall use the cylindrical coordinate system (r, θ, z) .

We assume that the mass density ρ is constant in the cylinder (cylindrical shell). The cylinder axis coincides with the crystalline axis z and the surfaces are stress free.

The strain-displacement relations are

$$\begin{aligned} \epsilon_{rr} &= \frac{\partial u_r}{\partial r} ; \quad \epsilon_{\theta\theta} = \frac{1}{r} \left(\frac{\partial u_\theta}{\partial \theta} + u_r \right) ; \quad \epsilon_{zz} = \frac{\partial u_z}{\partial z} ; \\ \epsilon_{r\theta} &= \frac{1}{2} \left(\frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} - \frac{u_\theta}{r} \right) ; \quad \epsilon_{\theta z} = \frac{1}{2} \left(\frac{\partial u_\theta}{\partial z} + \frac{\partial u_z}{\partial \theta} \right) ; \quad \epsilon_{rz} = \frac{1}{2} \left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r} \right) . \end{aligned} \quad (2)$$

The equations of motion are given now by

$$\begin{aligned}
\frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{1}{r} (\sigma_{rr} - \sigma_{\theta\theta}) &= \rho \frac{\partial^2 u_r}{\partial t^2} \\
\frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta\theta}}{\partial \theta} + \frac{\partial \sigma_{\theta z}}{\partial z} + \frac{2}{r} \sigma_{r\theta} &= \rho \frac{\partial^2 u_\theta}{\partial t^2} \\
\frac{\partial \sigma_{rz}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{\theta z}}{\partial \theta} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{1}{r} \sigma_{rz} &= \rho \frac{\partial^2 u_z}{\partial t^2} ,
\end{aligned} \tag{3}$$

where

$$\boldsymbol{\sigma} = \mathbf{C} \cdot \boldsymbol{\epsilon} . \tag{4}$$

The general solution of this problem, as we told before, must be performed numerically, but we shall consider now the particular case of the radial modes.

The radial modes are purely radial vibrations, so that $u_r \neq 0$ and $u_\theta = u_z = 0$. In the same way

$$\frac{\partial u_r}{\partial \theta} = \frac{\partial u_r}{\partial z} = 0 . \tag{5}$$

It can be shown that the second and third equations in (3) are satisfied automatically and we are left with

$$\frac{d^2 u_r}{dr^2} + \frac{1}{r} \frac{du_r}{dr} + (\beta_l^2 - \frac{\mu^2}{r^2}) u_r = 0 , \tag{6}$$

with $\beta_l^2 = \frac{\rho \omega^2}{C_{11}}$ and $\mu^2 = \frac{C_{22}}{C_{11}}$.

Eq.(6) is a Bessel equation of non-integer order. Thus we have the solution

$$u_r(r) = \begin{cases} A J_\mu(\beta_l r) + B J_{-\mu}(\beta_l r) , & \beta_l > 0 \\ A r + \frac{B}{r} , & \beta_l = 0 . \end{cases} \tag{7}$$

The boundary conditions at the surfaces are now

$$C_{11} \frac{du_r}{dr} + C_{12} \frac{u_r}{r} = 0 . \tag{8}$$

In the case of a thick cylinder, in order that u_r be finite at $r=0$, $B=0$. Thus we shall have:

$$u_r(r) = \begin{cases} AJ_\mu(\beta_l r) & , \beta_l > 0 \\ Ar & , \beta_l = 0 . \end{cases} \quad (9)$$

If $\sigma_{rr}(R)=0$, $A=0$ when $\beta_l=0$, and when $\beta_l > 0$ we have

$$C_{11}J'_\mu(\beta_l R) + C_{12}\frac{1}{R}J_\mu(\beta_l R) = 0 . \quad (10)$$

As

$$J'_\mu(\beta_l r) = \beta_l J_{\mu-1}(\beta_l r) - \frac{\mu}{r}J_\mu(\beta_l r) \quad (11)$$

eq.(10) becomes

$$C_{11}\beta_l J_{\mu-1}(\beta_l R) + (C_{12} - C_{11}\mu)\frac{1}{R}J_\mu(\beta_l R) = 0 , \quad (12)$$

thus giving

$$\beta_l R J_{\mu-1}(\beta_l R) = (\mu - \frac{C_{12}}{C_{11}})J_\mu(\beta_l R) . \quad (13)$$

This equation is a generalization of the expression obtained for an infinitely long isotropic cylinder²⁹

$$\beta_l J_0(\beta_l R) = \frac{1}{R} \frac{(1-2\nu)}{1-\nu} J_1(\beta_l R) \quad (14)$$

with the Poisson's factor $\nu = \frac{C_{12}}{2(C_{12} + C_{44})}$.

In the isotropic case $C_{11} = C_{22}$ and $C_{11} = C_{12} + 2C_{44}$. Thus it is easy to see that eq.(13) becomes in that case eq.(14).

In the case of the cylindrical shell, by using the boundary condition given in eq.(8), we obtain:

$$\begin{aligned} A(C_{11}J'_\mu(\beta_l r) + C_{12}\frac{1}{r}J_\mu(\beta_l r)) + B(C_{11}J'_{-\mu}(\beta_l r) + C_{12}\frac{1}{r}J_{-\mu}(\beta_l r)), \beta_l > 0 \\ A(C_{11} - C_{12}) - B(C_{11} - C_{12})\frac{1}{r^2}, \beta_l = 0 . \end{aligned} \quad (15)$$

As $\sigma_{rr}(a) = \sigma_{rr}(b)=0$, we must have $A = B=0$, for $\beta_l=0$, whereas for $\beta_l > 0$ we have

$$\begin{vmatrix} C_{11}\beta_l J'_\mu(\beta_l a) + C_{12}\frac{1}{a}J_\mu(\beta_l a) & C_{11}\beta_l J'_{-\mu}(\beta_l a) + C_{12}\frac{1}{a}J_{-\mu}(\beta_l a) \\ C_{11}\beta_l J'_\mu(\beta_l b) + C_{12}\frac{1}{b}J_\mu(\beta_l b) & C_{11}\beta_l J'_{-\mu}(\beta_l b) + C_{12}\frac{1}{b}J_{-\mu}(\beta_l b) \end{vmatrix} = 0 . \quad (16)$$

This is the dispersion relation for the elastic radial modes of an infinitely long cylindrical shell in the case of general anisotropy. In hexagonal crystals $C_{22} = C_{11}$ and $C_{12} = C_{11} - 2C_{66}$. Then the last equation reduces to eq.(33) in Ref.14, for the hexagonal crystals.

In the case of a thin shell it is possible to make an expansion to first order in $\frac{h}{a}$ in eq.(16). Then we arrive to

$$[(C_{12}^2 - C_{11}C_{22}) + C_{11}^2\beta_l^2 a^2]\beta_l a[2\mu J_\mu(\beta_l a)J_{-\mu}(\beta_l a) + \beta_l a J_\mu(\beta_l a)J_{-\mu-1}(\beta_l a) - \beta_l a J_{\mu-1}(\beta_l a)J_{-\mu}(\beta_l a)] = 0 . \quad (17)$$

Taking into account that

$$\begin{aligned} J'_\mu(\beta_l a) &= \beta_l J_{\mu-1}(\beta_l a) - \frac{\mu}{a}J_\mu(\beta_l a) \\ J'_{-\mu}(\beta_l a) &= \beta_l J_{-\mu-1}(\beta_l a) + \frac{\mu}{a}J_{-\mu}(\beta_l a) \end{aligned} \quad (18)$$

it can be seen that the factor involving the Bessel functions in eq.(17) is the Wronskian, having the value

$$J_\mu(\beta_l a)J'_{-\mu}(\beta_l a) - J'_\mu(\beta_l a)J_{-\mu}(\beta_l a) = -\frac{2\sin(2\pi)}{\pi\beta_l a} \neq 0 . \quad (19)$$

Thus the dispersion relation for the lowest breathing mode of a thin cylindrical shell of a general anisotropic crystal is given by

$$(C_{12}^2 - C_{11}C_{22}) + C_{11}^2\beta_l^2 a^2 = 0 , \quad (20)$$

which can be put in the form

$$\omega = \frac{1}{a}\sqrt{\frac{C_{11}C_{22} - C_{12}^2}{\rho C_{11}}} = \frac{2}{d}\sqrt{\frac{C_{11}C_{22} - C_{12}^2}{\rho C_{11}}} , \quad (21)$$

$d = 2a$ being the diameter.

In the case of hexagonal crystals $C_{22} = C_{11}$ and $C_{12} = C_{11} - 2C_{66}$ and eq.(21) reduces to

$$\omega = \frac{2}{a} \sqrt{\frac{C_{66}(C_{12} + C_{66})}{\rho(C_{12} + 2C_{66})}} \quad (22)$$

given in Ref.14.

For an isotropic crystal $C_{22} = C_{11}$ and $C_{12} = C_{11} - 2C_{44}$. Then eq.(21) reduces to

$$\omega = \frac{2}{a} \sqrt{\frac{C_{44}(C_{12} + C_{44})}{\rho(C_{12} + 2C_{44})}} \quad (23)$$

which coincides with the expressions given in Refs.11,14.

Eq.(21) is a simple analytic expression valid for all crystal systems. It provides in a quick way a first estimate of the lowest breathing mode frequency for nanowires. It was shown in Ref.14 that eq.(22) gave extremely good agreement with experimental and first principles theoretical values of the lowest breathing mode frequency of different nanotubes. It can be expected that the same will happen for eq.(21) when applied to other materials and crystal systems.

Eq.(16) gives the frequencies of higher order breathing modes.

III. CONCLUSIONS

We have obtained expressions in closed form for the dispersion relation of radial modes in infinitely long cylinders and cylindrical shells of general anisotropic materials. When considering the case of a very thin shell we arrive to a very simple analytic expression for the lowest breathing mode. This expression covers the cases of isotropic and hexagonal systems, previously given in the literature.

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- ¹ L. Pochhammer, Journal Rein. Angew. Math., **81**, 324 (1876)
- ² C. Chree, Q. J. Math., **22**, 287 (1886)
- ³ C. Chree, Trans. Camb. Philos. Soc., **14**, 250 (1889)
- ⁴ D. C. Gazis, J. Acoust. Soc. Am., **31**, 568 (1959); *ibid*, **31**, 573 (1959)
- ⁵ I. Mirsky, J. Acoust. Soc. Am., **36**, 41 (1964); *ibid*, **37**, 1016 (1965); *ibid*, **37**, 1022 (1965)
- ⁶ K. P. Soldatos, Appl. Mech. Rev., **47**, 501 (1994)
- ⁷ L. Elmaimouni, J. E. Lefebvre, V. Zhang and T. Gryba, Wave Motion, **42**, 177 (2005)
- ⁸ H. Ding, W. Chen, and L. Zhang, *Elasticity of Transversely Isotropic Materials* (Springer, Dordrecht, 2006)
- ⁹ M. A. Stroschio, and M. Dutta, *Phonons in Nanostructures* (Cambridge University Press, Cambridge, 2001)
- ¹⁰ H. Suzuura, and T. Ando, Phys. Rev. B, **65**, 235412 (2002)
- ¹¹ G. D. Mahan, Phys. Rev. B, **65**, 235402 (2002)
- ¹² L. Chico, R. Pérez-Alvarez, and C. Cabrillo, Phys. Rev. B, **73**, 075425 (2006)
- ¹³ M. Mitra, and S. Gopalakrishnan, J. Appl. Phys., **101**, 114320 (2007)
- ¹⁴ V. R. Velasco and M. C. Muñoz, Surf. Sci., **603**, 2950 (2009)
- ¹⁵ H. H. Demarest Jr., J. Acoust. Soc. Am., **49**, 768 (1971)
- ¹⁶ W. M. Vischer, A. Migliori, T. M. Bell and R. A. Reinert, J. Acoust. Soc. Am., **90**, 2154 (1991)
- ¹⁷ J. Maynard, Phys. Today, **49**, 26 (1996)
- ¹⁸ A. Migliori and J. Sarrao, *Resonant Ultrasound Spectroscopy*, (Wiley-Interscience, New York, 1997)
- ¹⁹ N. Nishiguchi, Y. Ando and M. N. Wybourne, J. Phys.: Condens. Matter, **9**, 5751 (1997)
- ²⁰ G. Li, G. A. Lamberton Jr. and G. R. Gladden, J. Appl. Phys., **104**, 033524 (2008)
- ²¹ N. Combe, P.-M. Chassaing and F. Demangeot, Phys. Rev. B, **79**, 045408 (2009)
- ²² D. Martínez-Gutiérrez and V. R. Velasco, Surf. Sci., **605**, 24 (2011)
- ²³ H. Lange, M. Mohr, M. Artemyev, U. Woggon and C. Thomsen, Nano Lett., **8**, 4614 (2008)
- ²⁴ S. O. Moriger, D. Khakhulin. H. T. Lemke, K. S. Kjaer, L. Guerin, L. Nuccio, C. B. Sorensen, M. M. Nielsen and R. Feidenhans, Nano Lett., **10**, 2461 (2010)
- ²⁵ L. Yang and M. Y. Chou, Nano Lett., **11**, 2618 (2011)

- ²⁶ C. Y. Wang and L. C. Zhang, *Nanotech.*, **19**, 075705 (2008)
- ²⁷ C. Y. Wang and L. C. Zhang, *Nanotech.*, **19**, 195704 (2008)
- ²⁸ S. S. Gupta and R. C. Batra, *Comput. Mater. Sci.*, **43**, 715 (2008)
- ²⁹ M. Hu, X. Wang, G. V. Hurtland, P. Mulvaney, J. P. Juste and J. E. Sader, *J. Am. Chem. Soc.*, **125**, 14925 (2003)